EDITOR: J. M. HONIG
ASSOCIATE EDITORS: J. W. RICHARDSON
W. R. ROBINSON

Journal of Solid State Chemistry

Volume 74, 1988

ACADEMIC PRESS, INC.
Harcourt Brace Jovanovich, Publishers
San Diego New York Boston
London Sydney Tokyo Toronto

Copyright © 1988 by Academic Press, Inc.
All rights reserved

No part of this publication may be reproduced or transmitted in any form or by any means, electronic or mechanical, including photocopying, recording, or any information storage and retrieval system, without permission in writing from the copyright owner.

The appearance of the code at the bottom of the first page of an article in this journal indicates the copyright owner's consent that copies of the article may be made for personal or internal use, or for the personal or internal use of specific clients. This consent is given on the condition, however, that the copier pay the stated per copy fee through the Copyright Clearance Center, Inc. (27 Congress Street, Salem, Massachusetts 01970), for copying beyond that permitted by Sections 107 or 108 of the U.S. Copyright Law. This consent does not extend to other kinds of copying, such as copying for general distribution, for advertising or promotional purposes, for creating new collective works, or for resale. Copy fees for pre-1988 articles are as shown on the article title pages; if no fee code appears on the title page, the copy fee is the same as for current articles.

0022-4596/88 $3.00

MADE IN THE UNITED STATES OF AMERICA

Contents of Volume 74

NUMBER 1, MAY 1988

LETTER TO THE EDITOR

A. K. GANGULI, L. GANAPATHI, J. GOPALAKRISHNAN, AND C. N. R. RAO. Low-Temperature Synthesis of Novel Layered Alkali Metal–MoO_3 Bronzes and Hexagonal Bronzes of the Type $K_yW_{1-x}Mo_xO_3$ 228

V. KRASNIKOV, M. VAIVADA, AND Z. KONSTANTS. Synthesis of Cerium Phosphates by Thermal Polycondensation of Mixtures CeO_2–$NH_4H_2PO_4$ and Investigation of Their Structure 1

D. F. MULLICA, HERBERT O. PERKINS, E. L. SAPPENFIELD, AND DAVID A. GROSSIE. Synthesis and Structural Study of Samarium Hexacyanoferrate (III) Tetrahydrate, $SmFe(CN)_6 \cdot 4H_2O$ 9

G. F. KHUDOROZHKO, I. P. ASANOV, A. V. MISCHENKO, L. N. MAZALOV, S. B. ERENBURG, V. E. FEDOROV, AND A. I. ROMANENKO. An X-Ray Photoelectron and X-Ray Emission Study of the Electronic Structure of Nb Trichalcogenides and Their Lithium Intercalates 16

CHRISTIAN ROBL AND WERNER F. KUHS. Complexes with Substituted 2,5-Dihydroxy-*p*-benzoquinones: A Neutron Diffraction Study of $BaC_6(C_6H_5)_2O_4 \cdot 4H_2O$ 21

G. POURROY, P. POIX, AND J. P. SANCHEZ. New Oxyfluoride Compounds $TaFeNiO_4F_2$ and $TaVNiO_4F_2$ 27

J. L. FOURQUET, F. PLET, AND Y. CALAGE. Crystal Structure and Magnetic Characterization of $(NH_4)_2FeF_5 \cdot H_2O$ 34

H. S. KILIAAN, F. P. VAN HERWIJNEN, AND G. BLASSE. The Luminescence of Ce^{3+}-Sensitized and Tb^{3+}-Activated Gadolinium Metaphosphates (GdP_3O_9–Ce,Tb) 39

B. ECH-CHAHED, F. JEANNOT, B. MALAMAN, ET C. GLEITZER. Préparation et étude d'une variété basse température de l'oxyphosphate de fer de valence mixte $\beta Fe_2(PO_4)O$ et de $NiCr(PO_4)O$: Un cas d'échange électronique rapide 47

P. D. BATTLE, T. C. GIBB, AND C. W. JONES. The Structural and Magnetic Properties of $SrMnO_3$: A Reinvestigation 60

W. LASOCHA, C. A. VOOS-ESQUIVEL, S. A. HODOROWICZ, B. Y. KIM, AND H. A. EICK. An X-Ray Powder Diffraction Study of the $YbCl_2$–YbI_2 System 67

M. GASGNIER, M.-O. RUALT, P. TREMBLAY, P. GOUGEON, M. POTEL, J. C. LEVET, AND H. NOEL. Macro- and Microstructural Analysis of $RBa_2Cu_3O_{7-x}$ (R = Y, Gd, Er, and Tm) Superconductor Thin Crystals between 300 and 15 K..... 74

EILEEN M. ANDREWS-ALLEN AND WILLIAM R. ROBINSON. Crystal Structures of a Cesium Iron(III) Phosphate, $Cs_3Fe_4(PO_4)_5$, and a Cesium Iron(III) Oxyphosphate, $Cs_7Fe_7(PO_4)_8O_2$ 88

NOBORU KIMIZUKA, TAKAHIKO MOHRI, YOSHIO MATSUI, AND KIITI SIRATORI. Homologous Compounds, $InFeO_3(ZnO)_m$ (m = 1–9) 98

M. PARRAS, M. VALLET-REGI, J. M. GONZÁLEZ-CALBET, M. ALARIO-FRANCO, AND J. C. GRENIER. Electron Microscopy and Diffraction of Barium–Lanthanum Ferrites: $Ba_xLa_{1-x}FeO_{3-y}$..... 110

YASUMICHI MATSUMOTO, KAZUYOSHI SUGIYAMA, AND EI-ICHI SATO. Improvement of $CaFe_2O_4$ Photocathode by Doping with Na and Mg..... 117

A. Wichainchai, P. Dordor, J. P. Doumerc, E. Marquestaut, M. Pouchard, P. Hagenmuller, and A. Ammar. On the Electrical Properties of Polycrystalline Delafossite-Type $AgNiO_2$ 126
L. Y. Zhang and W. E. Wallace. Hydrogenation Characteristics of the Isoelectronic Alloys $ZrMn_2$, ZrCrFe, and ZrVCo 132
E. Husson, A. Lachgar, and Y. Piffard. The Vibrational Spectra of the Layered Compounds $K_3Sb_3M_2O_{14},xH_2O$ (M = P, As): Normal Coordinate Analysis of $K_3Sb_3P_2O_{14},xH_2O$ 138
C. N. R. Rao. Solid-State Chemistry of High-Temperature Oxide Superconductors: The Experimental Situation 147
Yukio Hinatsu and Takeo Fujino. Magnetic Susceptibilities of UO_2–Pr_2O_3 Solid Solutions 163
H. Haeuseler, A. Cansiz, M. Himmrich, and M. Jung. Materials with Layered Structures: Crystal Structure of $Zn_{1.25}In_{2.5}S_3Se_2$, a New Polytype of $Zn_2In_2S_5$ and the Isotypic Compounds $Cd_{0.5}Ga_2InS_5$ and $Hg_{0.8}Ga_{1.6}In_{1.2}S_5$ 171
T. C. Gibb. An Investigation of Microdomains in $Ca_2LaFe_3O_{8+y}$ by Mössbauer Spectroscopy 176
T. Devanathan and T. K. K. Srinivasan. Raman Spectral Studies of Dehydration of $Cd(BrO_3)_2 \cdot 2H_2O$ 184
G. N. Kryukova, V. I. Zaikovskii, V. A. Sadykov, S. F. Tikhov, V. V. Popovskii, and N. N. Bulgakov. Study of the Nature of Extended Defects of Copper Oxide 191
V. A. Sadykov, S. F. Tikhov, G. N. Kryukova, N. N. Bulgakov, V. V. Popovskii, and V. N. Kolomiichuk. The Structure, Energetics, and Reactivity of Extended Defects of Copper Oxide 200
D. Hemeda et G. Tilloca. Nucléation et cristallisation dans un verre de chalcogénure du système As–Ge–Se en présence d'un agent nucléant 209

Number 2, June 1988

Letters to the Editor
M. Hervieu, C. Michel, A. Maignan, C. Martin, and B. Raveau. The 125 K Superconductor $Tl_{2-x}Ba_2Ca_2Cu_3O_{10+\delta}$: A Tentative Structural Model ... 428
A. F. Hepp, J. R. Gaier, J. J. Pouch, and P. D. Hambourger. Structural Chemistry of Au(III)-Substituted $Ba_2YCu_3O_{7-\delta}$ 433

D. J. Buttrey, P. Ganguly, J. M. Honig, C. N. R. Rao, R. R. Schartman, and G. N. Subbanna. Oxygen Excess in Layered Lanthanide Nickelates 233
W. P. Zhang, K. H. Kuo, Y. F. Hou, and J. Z. Ni. Direct Observation of Molecular Images of Lanthanide Phthalocyanines. I. Molecular, Crystal, and Twin Structures 239
S. Horiuchi, F. Izumi, T. Mitsuhashi, K. Uchida, T. Shimomura, and K. Ogasahara. Structural Studies of β-Bi_2O_3 Stabilized by the Addition of PbF_2 247
Roger Frech and Enzo Cazzanelli. Vibrational Study of Selenate-Doped Lithium Sulfate: Single Crystals and Fused Salts 256

U. D. Scholz, W. Jeitschko, and M. Reehuis. The Polyphosphides $NbMn_2P_{12}$, $MoMn_2P_{12}$, and WMn_2P_{12} with $TiMn_2P_{12}$-Type Structure 260
F. J. Lincoln, J. R. Sellar, and B. G. Hyde. A New Examination of the Thermodynamic Properties of the Oxygen-Deficient Fluorite-Type Phase α-$PrO_{2-\delta}$ ... 268
Han Wan Shu, S. Jaulmes, et J. Flahaut. Système As–Ge–Te. III. Étude cristallographique d'une famille de composés a modèles structuraux communs: β-As_2Te_3, As_4GeTe_7, et $As_2Ge_nTe_{3+n}$ (n = 1 à 5) 277
A. C. W. P. James and J. B. Goodenough. Structure and Bonding in Lithium Ruthenate, Li_2RuO_3 287
Andrée Kahn, Tomé Gbehi, Jeanine Thery, and Jean-Jacques Legendre. Short-Range Order in Barium Hexaaluminate (Phase I) Single Crystals..... 295
D. W. Jones, I. J. McColm, J. Yerkess, and N. J. Clark. Carbon Species in the Crystal Structures of Uranium-Transition-Element Carbides, UMC_2 304
K. K. Stavrev, K. D. Kynev, and G. St. Nikolov. Vibronic Spectra Analysis of Transition-Metal Ion Impurity Centers in II–VI Compounds 314
C. Manolikas. New Results on the Phase Transformations of In_2Se_3..... 319
M. Taïbi, J. Aride, E. Antic-Fidancev, M. Lemaitre-Blaise, P. Porcher, and P. Caro. The Optical Properties of Lanthanides in the Ln_2BaZnO_5 Area of the Mixed Oxide System Ln–Ba–Zn–O 329
Mohamed Faouzi Zid, Tahar Jouini, Noureddine Jouini, et Mohamed Omezzine. Préparation et structure cristalline de $K_2Nb_2As_2O_{11}$ 337
Georges Dénès. $PbSn_4F_{10}$: A New Disordered Fluorite-Type Fast Ion Conductor 343
Zoltan Blum, Sven Lidin, and Ronnie Thomasson. Zeolites: Conveyers of Non-Euclidean Geometry 353
Jean Galy, Renée Enjalbert, Patrice Millet, Christophe Faulmann, and Patrick Cassoux. Structural Systematics around High T_c Superconductors $YBa_2Cu_3O_{6+x}$ 356
Om Parkash, Ch. Durga Prasad, and Devendra Kumar. Defect Structure and Electrical Properties of Magnesium-Substituted Strontium Titanate 369
A. El Jazouli, C. Parent, J. M. Dance, G. Le Flem, P. Hagenmuller, and J. C. Viala. $Na_4Nb(PO_4)_3$, a Material with a Reversible Crystal–Glass Transformation: Structural and Optical Comparison 377
J. T. S. Irvine and A. R. West. Solid Electrolytes Based on Na_3PO_4: M^{4+} (M = Zr, Hf, Ti, Sn, Ce, Th)..... 385
Yukio Hinatsu and Takeo Fujino. Magnetic Susceptibilities of $Ca_yU_{1-y}O_{2+x}$ Solid Solutions 393
Osamu Tamada, Naoichi Yamamoto, and Yoshio Oka. Hydrothermal Synthesis and Structure Determination of a New Manganese (III) Oxide, $BaMn_2O_3(OH)_2$..... 401

Brief Communications
S. L. Wang, C. C. Wang, and K. H. Lii. $Mo_3P_5SiO_{19}$: A Molybdenum Phosphate Containing a Confacial Bioctahedral Molybdenum(III) Dimer with a Mo–Mo Bond..... 409
M. M. Thackeray and A. De Kock. Synthesis of γ-MnO_2 from $LiMn_2O_4$ for Li/MnO_2 Battery Applications 414

D. F. MULLICA, H. O. PERKINS, AND E. L. SAPPENFIELD. A Structural Investigation of Monoclinic $SmCo(CN)_6 \cdot 4H_2O$ 419
G. SEKAR, V. RAMAKRISHNAN, AND G. ARULDHAS. IR and Polarized Raman Spectra of $(NH_4)_2M(SO_4)_2 \cdot 6H_2O$ (M = Zn, Mn) 424

BOOK REVIEWS
GARY WNEK. *Conducting Polymers: Special Applications*. Edited by Luis Alcacer 438
ROLAND VON BALLMOOS. *Studies in Surface Science and Catalysis, Vol. 33, Synthesis of High-Silica Aluminosilicate Zeolites*. By. P. A. Jacobs and J. A. Martens 438

ANNOUNCEMENTS 440

AUTHOR INDEX FOR VOLUME 74 441

The Subject Index for Volume 74 will appear in the December 1988 issue as part of a cumulative index for the year 1988.

Information for Authors

The *Journal of Solid State Chemistry* is a research journal devoted to the chemical, structural, thermodynamic, electronic, magnetic, and optical properties and processes of solids. Theoretical and experimental contributions are both welcome. Critical reviews are occasionally presented in selected rapidly developing fields. The journal also carries a Letters Section.

Original papers only will be considered. Manuscripts are accepted for review with the understanding that the same work has not been and will not be nor is presently submitted elsewhere, and that its submission for publication has been approved by all of the authors and by the institution where the work was carried out; further, that any person cited as a source of personal communications has approved such citation. Written authorization may be required at the Editor's discretion. Articles and any other material published in the *Journal of Solid State Chemistry* represent the opinions of the author(s) and should not be construed to reflect the opinions of the Editor(s) and the Publisher.

Authors submitting a manuscript do so on the understanding that if it is accepted for publication, copyright in the article, including the right to reproduce the article in all forms and media, shall be assigned exclusively to the Publisher. The Publisher will not refuse any reasonable request by the author for permission to reproduce any of his or her contributions to the journal.

Manuscripts may be presented as articles (i.e., conventional full-length expositions), or notes (brief rapid communications of important new work) which are limited to 1200 words. English, French, and German are the official languages of the Journal but submission of articles in English is encouraged. Manuscripts should be submitted to *Journal of Solid State Chemistry,* Editorial Office, Seventh Floor, 1250 Sixth Avenue, San Diego, California 92101.

Manuscripts should be submitted in quadruplicate—double-spaced on one side of 21.5 × 28 cm paper. Headings of major sections should be typed in capital letters and centered on the page. Each page of the manuscript should be numbered. Page one should consist of the manuscript title, the author's name, and the author's affiliation. For multiple authors, the author to whom correspondence is to be addressed should be indicated. Page two should consist of an abstract (50–150 words) suitable for use in *Chemical Abstracts.* The American Chemical Society's *Style Guide* or the *Style Manual* of the American Institute of Physics should be followed regarding matters of style and abbreviation.

Tables. Tables should be numbered with Roman numerals in a sequence corresponding to the order of citation in the text. Footnotes to tables are to be placed directly below the table and should be indicated by superscript, lowercase italic letters (^{a,b,c}). Tables longer than two manuscript pages should be submitted as clear, sharp glossy photographs. They will be reproduced by photoreproduction and should be designed to fit the Journal page after 50% reduction in each dimension. Errors in such tables cannot be corrected in proof.

Auxiliary Material. In lieu of publication, unusually long tables and sequences of repetitive figures must be deposited with the National Auxiliary Publications Service (NAPS).

For material to be deposited, a deposit fee of $25.00 for up to 98 pages of standard-size or 49 pages of oversize deposited material is to be paid by the authors to NAPS. Appropriate transmittal forms to accompany the deposited material are supplied to the authors by the Editor at the time a paper is accepted for publication. The following footnote (wherein missing numbers are to be inserted by the author in page proof) should be used to reference deposited material.

See NAPS document No. ___ for ___ pages of supplementary material. Order from ASIS/NAPS. Microfiche Publications, P.O. Box 3513, Grand Central Station, New York, NY 10163. Remit in advance $4.00 for microfiche copy or for photocopy, $7.75 up to 20 pages plus $.30 for each additional page. All orders must be prepaid. Institutions and Organizations may order by purchase order. However, there is a billing and handling charge for this service of $15. Foreign orders add $4.50 for postage and handling, for the first 20 pages, and $1.00 for additional 10 pages of material, $1.50 for postage of any microfiche orders.

Figures. Figures should be submitted as glossy prints or as original black ink drawings, no larger than 21.5 × 28 cm. Press type is not acceptable. It is important that lettering on drawings be done with a lettering set and be planned to fit the proportion of the printed page. Lettering on the original should be large enough to be legible after reduction of the figure to single-column width. The difference in type size within a figure should be no more than approximately 15%. The caption of each axis should be lettered parallel to its axis. Background grids should not be included. For halftone reproductions, glossy, high-contrast, black and white prints should be submitted.

Illustrations in color can be accepted only if the authors defray the cost. Each figure should be identified on the back with the author's name and figure number. Figures are to be cited in the text by consecutive Arabic numerals. Figure captions should be typed as a list on a separate page.

Equations. Equations should be typewritten or clearly handwritten with an Arabic number if necessary for reference placed in parentheses to the right of equation. Reference to equations should use the form "Eq. (3)."

Footnotes. Footnotes to the text should be indicated by consecutive superscript numbers and listed on a separate page at the end of the paper.

References. References should be cited in the text by consecutive underlined numbers in parentheses. The references must appear on a separate sheet, listed in numerical order, i.e., in accordance with order of citation in the text. After the reference number, the author's initials, last name, journal name, volume, initial page number, and year (in parentheses) should be listed in that order. Abbreviations for journal names should follow the style of *Chemical Abstracts Service Source Index*, 1985. For book references, give the author's name, name of book (in quotes), Editor's name (if any), edition (if other than the first), chapter or page number, publisher's name, place and year of publication.

Manuscripts Dealing Primarily with Single-Crystal Structure. The *abstract* should contain the chemical formula, crystal system, and space group (Hermann–Mauguin symbol), lattice constants with esd's, Z, and significant structural features.

The *experimental* section should contain the following information in as brief a form as possible: chemical formula, source of material and its color, lattice constants with esd's, wavelength of the radiation used in their calculation, temperature at which they were measured, type of filter or monochromator, possible space groups (and method of distinguishing between groups with the same absences), Z, crytstal dimensions, absorption coefficient, method of correcting for absorption, type of data collection, number of reflections measured, number of independent reflections, and agreement factors between multiply measured or equivalent reflections. The description of the structure determination and refinement should indicate a brief outline of the method used, sources of f, $\Delta f'$, and $\Delta f''$, final R factors (weighted and unweighted), the function minimized in refinement, the form of weights in the refinement, and the extinction correction (if applied).

Structural results should contain a description of the structure and the following tables: a table of all atomic coordinates (with esd's) and important bond distances and angles (with esd's). In those structures where atomic displacements or atomic motion is important (ionic conductors, superlattice structures solved as a substructure, phase changes, etc.), it may be appropriate to add a table of anisotropic temperature factors. When submitting a manuscript three copies of a listing of h, k, l, F_o, F_c (σF_o is optional) must be provided for the reviewers and also, if not included in the manuscript, three copies of a table of temperature factors. Authors are strongly encouraged to deposit with NAPS structure factor tables, tables of anisotropic temperature factors, all nonessential bond distances and angles, and other supporting structural detail; such material will be retained in the *Journal's* editorial office for no longer than one year after publication of the article.

Letters to the Editor. Letters to the Editor will be accepted for publication subject to approval by the communicators, who upon their recommendation for acceptance will forward the manuscript directly to the Editorial Office. Each article should indicate clearly the novelty and urgency of the contribution; it may be helpful to document this more explicitly in an accompanying letter of transmittal. Each communicator must satisfy himself that the content is not only scientifically sound, but also likely to have such impact as to merit rapid publication. Accepted manuscripts will be published on an accelerated publication schedule. The author will not receive proofs for correction; it is the responsibility of the author to ensure that the manuscript as submitted is free of typographical or substantive errors. Letters should be no longer than 1200 words, with an absolute minimum of figures, tables, and references; an abstract not exceeding 150 words should also be provided. Manuscripts should be sent to the Editor, an Associate Editor, or to one of the following members of the Editorial Advisory Board: E. F. Bertaut, J. B. Goodenough, P. Hagenmuller, A. Rabenau, C. N. R. Rao, or A. Wold. Full addresses for these Board members are listed on the inside front cover of the journal.

Book Reviews. Book Reviews are published on an irregular schedule, and are limited to books whose content bears directly on the general area of solid state chemistry. Reviews should be submitted directly to the Editor for Book Reviews, Dr. Edward Kostiner, Department of Chemistry and Institute of Materials Science, University of Connecticut, Storrs, Connecticut 06268.

Proofs. Unfolioed page proofs will be sent directly to the author from the printer together with order forms for reprints. There is no page charge.